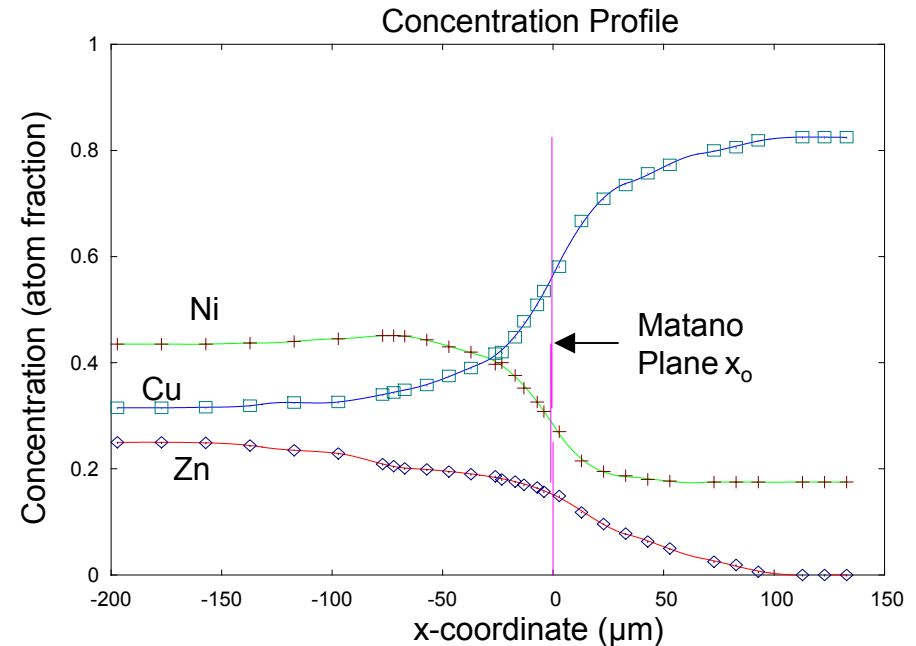# *Multi*DiFlux Program - Version 1.1
Analysis of Single-phase Ternary Diffusion Couples
M.A. Dayananda, Purdue University —DMR-0304777

The phenomenon of interdiffusion plays a major role in the development and stability of microstructures in multicomponent, multiphase alloy assemblies, ranging from high temperature alloys, coatings, claddings, thin films to nuclear fuels and nuclear wastes. To understand the diffusion structure development, one needs to determine interdiffusion coefficients as functions of compositions in individual phases. The *Multi*DiFlux (version 1.1) is a user-friendly computer program developed for the evaluation of interdiffusion fluxes and ternary interdiffusion coefficients from a single-phase diffusion couple over selected composition ranges in the diffusion zone. An application of the program to the analysis of a Cu-Ni-Zn diffusion couple annealed at 775°C for 48 hours is presented here.

Concentration Profile

Above: Concentration profiles fitted to the experimental data and the Matano plane calculated by the MultiDiFlux program.
Below: Ternary interdiffusion coefficients (in units of m^2/s) calculated for ranges on either side of the Matano Plane x_o.

Range	$\widetilde{D}_{Zn\,Zn}^{Cu}$	$\widetilde{D}_{Zn\,Ni}^{Cu}$	$\widetilde{D}_{Ni\,Zn}^{Cu}$	$\widetilde{D}_{Ni\,Ni}^{Cu}$
-∞ to x_o	1.56E-14	-6.51E-17	-6.1E-15	2.03E-15
x_o to +∞	6.0E-15	4.41E-16	-3.96E-17	1.19E-15

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Education:

Kevin M. Day, a Ph.D student, is involved in the use and testing of the *Multi*DiFlux program. Dr. L. Ramdas Ram-Mohan of Quantum Semiconductor Algorithms has been an active consultant and contributor to the development of the computer code. The program is currently being modified and extended to handle diffusion problems relevant to multiphase ternary systems through the current NSF support.

Outreach:

The *Multi*DiFlux program was presented in a NIST workshop on the analysis of multicomponent, multiphase diffusion held in March 2003. A current version of the program modified through NSF support is made available for downloading as a free educational and research tool for diffusion studies of single phase systems at the site: https://engineering.purdue.edu/MSE/Fac Staff/Faculty/dayananda.wshtml . Kevin Day will be presenting an application of the program to ternary diffusion couples at the Materials Science & Technology meeting to be held during November 9-12, 2003 in Chicago.